

# Photonuclear Benchmarks with a Comparison of COG and MCNPX Results

*David P. Heinrichs and Edward M. Lent*

U.S. Department of Energy

Lawrence  
Livermore  
National  
Laboratory

This paper was submitted to the Cross Section Evaluation Working Group (CSEWG) at the Meeting held at Brookhaven National Laboratory, November 4 - 6, 2003.

**October 15, 2003**

## DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

This report has been reproduced  
directly from the best available copy.

Available to DOE and DOE contractors from the  
Office of Scientific and Technical Information  
P.O. Box 62, Oak Ridge, TN 37831  
Prices available from (423) 576-8401  
<http://apollo.osti.gov/bridge/>

Available to the public from the  
National Technical Information Service  
U.S. Department of Commerce  
5285 Port Royal Rd.,  
Springfield, VA 22161  
<http://www.ntis.gov/>

OR

Lawrence Livermore National Laboratory  
Technical Information Department's Digital Library  
<http://www.llnl.gov/tid/Library.html>

## The IAEA Photonuclear Data Library

The Nuclear Data Section of the International Atomic Energy Agency (IAEA) has distributed an evaluated photonuclear data library [1] in standard ENDF-6 format that is intended for use in transport codes. This “IAEA Photonuclear Data Library” consists of a number of individual ASCII text files for various elements that have been recently processed into the single binary (COG data library) file “COGPNUC” with corresponding changes to the COG code for use in transport calculations involving photonuclear reactions [2].

## Barber and George Benchmark Experiments

Barber and George [3] have measured the total neutron yields produced by the bombardment of thick targets of C, Al, Cu, Ta, Pb, and U by mono-energetic beams of electrons. They estimated the absolute accuracy of their experimental measurements to be  $\pm 15\%$ .

## COG Benchmark Model Details

Barber and George reported the target thicknesses as areal densities (in  $\text{g}/\text{cm}^2$ ). The thicknesses (in cm) are calculated for each target using the reported areal density and the assumed density as given in Table 1.

Table 1. Reported and Calculated Target Thicknesses

Target	Density	Thickness	
C-I	1.70 $\text{g}/\text{cm}^3$	38.91 $\text{g}/\text{cm}^2$	22.8882 cm
Al-I	2.70 $\text{g}/\text{cm}^3$	24.19 $\text{g}/\text{cm}^2$	8.9593 cm
Cu-A	8.92 $\text{g}/\text{cm}^3$	1.372 $\text{g}/\text{cm}^2$	0.1538 cm
Cu-I	8.92 $\text{g}/\text{cm}^3$	13.26 $\text{g}/\text{cm}^2$	1.4866 cm
Cu-II	8.92 $\text{g}/\text{cm}^3$	26.56 $\text{g}/\text{cm}^2$	2.9776 cm
Cu-III	8.92 $\text{g}/\text{cm}^3$	39.86 $\text{g}/\text{cm}^2$	4.4686 cm
Cu-IV	8.92 $\text{g}/\text{cm}^3$	53.13 $\text{g}/\text{cm}^2$	5.9563 cm
Ta-1	16.6 $\text{g}/\text{cm}^3$	6.21 $\text{g}/\text{cm}^2$	0.3741 cm
Pb-I	11.34 $\text{g}/\text{cm}^3$	5.88 $\text{g}/\text{cm}^2$	0.5185 cm
Pb-II	11.34 $\text{g}/\text{cm}^3$	11.42 $\text{g}/\text{cm}^2$	1.0071 cm
Pb-III	11.34 $\text{g}/\text{cm}^3$	17.30 $\text{g}/\text{cm}^2$	1.5256 cm
Pb-IV	11.34 $\text{g}/\text{cm}^3$	22.89 $\text{g}/\text{cm}^2$	2.0185 cm
Pb-VI	11.34 $\text{g}/\text{cm}^3$	34.42 $\text{g}/\text{cm}^2$	3.0353 cm
U-I	18.95 $\text{g}/\text{cm}^3$	6.17 $\text{g}/\text{cm}^2$	0.3256 cm
U-II	18.95 $\text{g}/\text{cm}^3$	12.42 $\text{g}/\text{cm}^2$	0.6554 cm
U-III	18.95 $\text{g}/\text{cm}^3$	18.61 $\text{g}/\text{cm}^2$	0.9821 cm

Each target is modeled as a 4.5'' x 4.5'' parallelepipedon with the thickness given in Table 1. The source is specified as a mono-energetic electron beam distributed uniformly throughout a 0.5''-diameter disc centered on one of the 4.5'' x 4.5'' faces of the parallelepipedon and directed inward perpendicularly to the plane of the surface. A vacuum boundary condition is applied to the surface of the parallelepipedon and thus particle transport only takes place in one medium.

Coupled electron, photon and neutron transport COG [4] calculations were performed using version 10.171 on the GPS machines. To enable photonuclear reactions the user must specify "basic electron photon neutron photonuclear" in the COG "basic block" of each input file. The numbers of neutrons (and other particles) that escape the target were counted by specifying a "boundary-crossing detector" with "particle counting" on the surface of the parallelepipedon. A sample COG input listing is provided in Appendix A.

## Results of Benchmark Calculations

Table 2 lists the target, the energy of the electron beam and the experimentally measured [3], [5] and calculated neutron yield per million incident electrons. The MCNPX calculational results were run to high precision and are those reported recently by researchers at Los Alamos [5]. The COG results are those of the authors and are based on simulations of one million electron histories for electrons above 1.0 MeV. The results are also provided in graphical form in Appendix B.

Table 2. Experimental and Calculated Neutron Yields from Electron Bombardment

Material	Electron Beam	Neutron Yield per 10 <sup>6</sup> Electrons		
Target	Energy	Experiment	MCNPX	COG
C-I	26.0 MeV	31 ± 5	20	27 ± 1
	28.3 MeV	60 ± 9	45	54 ± 2
	34.4 MeV	173 ± 26	140	155 ± 3
Al-I	22.2 MeV	46 ± 7	35	37 ± 1
	28.3 MeV	210 ± 32	158	162 ± 1
	34.3 MeV	430 ± 65	329	332 ± 2
Cu-A	13.9 MeV	1.1 ± 0.2	0.6	0.8 ± 0.1
	16.3 MeV	3.6 ± 0.5	2.8	3.1 ± 0.2
	19.9 MeV	11.8 ± 1.8	8.6	9.1 ± 0.5
	23.5 MeV	21.1 ± 3.2	14.0	15.9 ± 0.6
	25.9 MeV	26.3 ± 3.9	17.2	18.4 ± 0.7
	28.2 MeV	30.9 ± 4.6	19.7	20.0 ± 0.7
	31.9 MeV	35.8 ± 5.4	22.6	24.2 ± 0.7
Cu-I	16.1 MeV	30 ± 5	39	44 ± 1
	21.2 MeV	260 ± 39	260	279 ± 3
	28.3 MeV	820 ± 123	739	772 ± 4
	34.4 MeV	1290 ± 194	1128	1166 ± 5
	35.5 MeV	1390 ± 209	1189	1245 ± 5

Table 2. Experimental and Calculated Neutron Yields from Electron Bombardment (cont.)

Cu-II	16.1 MeV	$50 \pm 8$	66	$73 \pm 1$
	21.2 MeV	$430 \pm 65$	446	$483 \pm 3$
	28.3 MeV	$1390 \pm 209$	1325	$1387 \pm 6$
	34.4 MeV	$2370 \pm 356$	2117	$2221 \pm 7$
Cu-III	16.1 MeV	$70 \pm 11$	83	$94 \pm 1$
	21.2 MeV	$530 \pm 80$	562	$602 \pm 4$
	28.3 MeV	$1800 \pm 270$	1688	$1784 \pm 6$
	34.4 MeV	$2930 \pm 440$	2729	$2873 \pm 8$
Cu-IV	16.1 MeV	$100 \pm 15$	94	$105 \pm 1$
	21.2 MeV	$600 \pm 90$	634	$677 \pm 4$
	28.3 MeV	$2130 \pm 320$	1910	$1989 \pm 7$
	34.4 MeV	$3350 \pm 503$	3104	$3241 \pm 8$
Ta-I	10.3 MeV	$80 \pm 12$	8.2	$7.5 \pm 0.2$
	18.7 MeV	$520 \pm 78$	578	$544 \pm 5$
	28.3 MeV	$1380 \pm 207$	1433	$1362 \pm 7$
	34.3 MeV	$1810 \pm 272$	1726	$1655 \pm 8$
Pb-I	18.7 MeV	$730 \pm 110$	627	$569 \pm 3$
	28.3 MeV	$1690 \pm 254$	1366	$1298 \pm 5$
	34.5 MeV	$2120 \pm 318$	1611	$1536 \pm 5$
Pb-II	18.7 MeV	$1320 \pm 198$	1135	$1051 \pm 5$
	28.3 MeV	$3450 \pm 518$	2871	$2731 \pm 7$
	34.5 MeV	$4720 \pm 708$	3717	$3575 \pm 8$
Pb-III	18.7 MeV	$1770 \pm 266$	1503	$1395 \pm 5$
	28.3 MeV	$4690 \pm 704$	3953	$3792 \pm 8$
	34.5 MeV	$6460 \pm 969$	5264	$5099 \pm 9$
Pb-IV	18.7 MeV	$2100 \pm 317$	1748	$1645 \pm 6$
	28.3 MeV	$5370 \pm 806$	4668	$4506 \pm 9$
	34.5 MeV	$7770 \pm 1166$	6290	$6114 \pm 10$
Pb-VI	18.7 MeV	$2500 \pm 375$	2053	$1933 \pm 6$
	28.3 MeV	$6670 \pm 1000$	5556	$5381 \pm 9$
	34.5 MeV	$9000 \pm 1350$	7575	$7387 \pm 10$
U-I	16.4 MeV	$1070 \pm 161$	N/A	$1029 \pm 7$
	21.1 MeV	$2330 \pm 350$	N/A	$2161 \pm 10$
	28.4 MeV	$3860 \pm 579$	N/A	$3268 \pm 12$
	35.5 MeV	$4880 \pm 732$	N/A	$3802 \pm 14$
U-II	16.4 MeV	$1950 \pm 293$	N/A	$1907 \pm 9$
	21.1 MeV	$4310 \pm 647$	N/A	$4229 \pm 14$
	28.4 MeV	$7850 \pm 1178$	N/A	$7143 \pm 18$
	35.5 MeV	$10735 \pm 1610$	N/A	$9229 \pm 21$

Table 2. Experimental and Calculated Neutron Yields from Electron Bombardment (cont.)

U-III	11.5 MeV	$380 \pm 57$	N/A	$326 \pm 3$
	16.4 MeV	$2530 \pm 380$	N/A	$2536 \pm 11$
	21.1 MeV	$5900 \pm 885$	N/A	$5676 \pm 17$
	28.4 MeV	$10460 \pm 1569$	N/A	$9814 \pm 22$
	35.5 MeV	$14940 \pm 2241$	N/A	$13175 \pm 25$

### Detailed Remarks

Graphite: The COG results are in very good agreement with the measurements of Barber and George for graphite. Note that MCNPX under-predicts the neutron yield slightly for these measurements. Aluminum: COG and MCNPX results are in good agreement with each other but both codes under-predict the neutron yield by nearly 25%. Copper: COG and MCNPX are in good agreement with each other but both codes under-predict the neutron yields of the thinnest target (Cu-A) by as much as 35%. Tantalum: COG and MCNPX are in excellent agreement with measurement for incident electron energies above 18 MeV. However, both codes under-predict the neutron yield at low energy by an order of magnitude. Lead: COG and MCNPX are in good agreement with each other but both codes under-predict the neutron yields of the thinnest targets (Pb-I and Pb-II) by as much as 30%. Uranium: COG results are in good agreement with measurement.

### Conclusion

COG (and MCNPX) calculated neutron yields are generally in good agreement with the measurements of Barber and George with one (minor) over-predicted yield (see Cu-I) but users are cautioned that calculated yields may be under-predicted by as much as 35% (see Cu-A) or by an order-of-magnitude at very low energies near the reaction threshold (see Ta-I). Nonetheless, these results validate COG for use with the IAEA Photonuclear Data Library (COGPNUC) as another state-of-the-art computational method (such as MCNPX) for simulating neutron production in C, Al, Cu, Ta, Pb, and U due to photonuclear reactions.

### References

- [1] P. Oblozinsky et al., "Handbook on photonuclear data for applications, Cross sections and Spectra", IAEA-TECDOC-Draft No 3, March 2000.
- [2] Edward M. Lent, personal communication.
- [3] W. C. Barber and W. D. George, "Neutron Yields from Targets Bombarded by Electrons", *Physical Review*: 116 (6) 1551 – 1559, December 15, 1959.
- [4] Richard M. Buck, Edward M. Lent, Tom Wilcox and Stella Hadjimarkos, "COG User's Manual, A Multiparticle Monte Carlo Transport Code", Fifth Edition.

- [5] M. C. White, R. C. Little, M. B. Chadwick, P. G. Young, and R. E. MacFarlane, “Photonuclear Physics in Radiation Transport – II: Implementation”, *Nuclear Science and Engineering*: 144, 174 – 189 (2003).

### **Acknowledgements**

The authors are pleased to acknowledge the contribution of Dr. Richard M. Buck who assisted us in creating the electron cross-section libraries. This work was performed under the auspices of the U.S. Department of Energy by the University California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

## Appendix A

### *Sample COG Input Listing*

16.4 MeV electrons on the U-I Target

```
$ -----
$ Physical Review: 116(6)1551-1559(1959), "Neutron Yields from Targets Bombarded
$ by Electrons", W. C. Barber and W. D. George (Stanford University).
$
$ Nuclear Science and Engineering: 144,174-189(2003), "Photonuclear Physics in
$ Radiation Transport - II: Implementation", M. C. White, R. C. Little, M. B.
$ Chadwick, P. G. Young and R. E. MacFarlane (LANL).
$ -----
basic
  electron photon neutron photonuclear
source
  npart=1E+6 nofile
  define position = 1 ss-disk -0.1628 0 0 0 0 0.635 $ 0.5" diameter beam spot
  define energy   = 1 electron line 16.4 1
  define time     = 1 steady
  define angle    = 1 1 0 0 fixed
  increment 1 position=1 energy=1 time=1 angle=1
mix nlib=ENDFB6R7
  mat=1 a-f 18.95 u234 0.005 u235 0.720 u238 0.99275
assign
  1 1 1 1.0 2 0 2 1.0
egs
  pegslib=/g/g12/u381872/runPEGS4/U.dat $ PEGS4 (U) library file on GPS
  esectors = 1
  ecut 1.0
geometry
  sector 1 U-I -1
  sector 2 Void 1 -2
  boundary vacuum 2
surfaces
  1 box 0.3256 11.43 11.43 $ Thickness = (6.17 g/sq.cm)/(18.95 g/cc)
  2 box 0.4 12. 12.
detector
  number=#0000001 title="number of leakage neutrons per incident electron"
  boundary counts 1 2 276.176 $ = [4(0.3256) + 2(11.43)](11.43)
end
```

## **Appendix B**

### *Graphs of the Results*











